

WHAT IS CLAIMED IS:

Sub A2 } 1. A molecular reaction characteristic predicting method for predicting a reaction characteristic of a molecule, said method comprising the steps of:

setting a molecule surrounding surface so as to be reflected in a spatial dimension of a molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces;

assuming that a portion of each of said component surrounding surfaces on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces, and predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said component spaces.

2. A molecular reaction characteristic predicting method as set forth in claim 1, wherein said molecule surrounding surface is an outermost contour enveloping surface formed by a plurality of atomic spherical surfaces, each of which extends around the center of each of said atoms of said molecule.

3. A molecular reaction characteristic predicting method as set forth in claim 1, wherein each of said component spaces is a space surrounding each of said atoms of said molecule.

4. A molecular reaction characteristic predicting method as set forth in claim 3, wherein each of atomic spherical surfaces is derived so as to extend around the center of each of said atoms of said molecule, and wherein it is assumed that a portion of each of said atomic spherical surfaces intersecting other atomic spherical surfaces is an interior spherical surface and that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier spherical surface, each of said component spaces being a space surrounded by a surface, which cuts said interior spherical surface, and said frontier spherical surface.

5. A molecular reaction characteristic predicting method as set forth in claim 1, wherein each of atomic spherical surfaces is derived so as to extend around the center of each of said atoms of said molecule, and wherein it is assumed that a portion of each of said atomic spherical surfaces intersecting other atomic spherical surfaces is an interior spherical surface and that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier spherical surface, said frontier surrounding surface being said frontier spherical

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surface.

6. A molecular reaction characteristic predicting method as set forth in claim 1, wherein each of atomic spherical surfaces is derived so as to extend around the center of each of said atoms of said molecule, and wherein each of said atomic spherical surfaces is a spherical surface having a van der Waals radius of each of said atoms or a radius which is obtained by commonly adding a predetermined thickness to said van der Waals radius of each of said atoms.

7. A molecular reaction characteristic predicting method as set forth in claim 1, wherein said molecule surrounding surface is a surrounding surface which surrounds a space formed by the frontier molecular orbital of said molecule.

8. A molecular reaction characteristic predicting method as set forth in claim 1, wherein said predetermined space dividing procedure comprises the Voronoi division of said molecule surrounding space using the center of each of said atoms of said molecule as a mother point, and each of said component spaces is a Voronoi region formed by said Voronoi division.

9. A molecular reaction characteristic predicting method as set forth in claim 1, wherein said space occupied rate is based on a volume of each of said component spaces.

10. A molecular reaction characteristic predicting method as set forth in claim 1, wherein said space occupied rate is based on the number of said probe points existing on said frontier surrounding surface.

11. A molecular reaction characteristic predicting method as set forth in claim 1, wherein said space occupied rate is based on an area of said frontier surrounding surface.

12. A molecular reaction characteristic predicting method as

set forth in claim 1, wherein said electrostatic factor is normalized by dividing said sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces by said space occupied rate of said corresponding one of said component spaces, and said steric factor is normalized by dividing said sum of said van der Waals energies on said frontier surrounding surface of a corresponding one of said component spaces by said space occupied rate of said corresponding one of said component spaces.

13. A molecular reaction characteristic predicting method as set forth in claim 1, wherein said probe atom is an sp^3 carbon, an sp^2 carbon or an sp carbon.

14. A molecular reaction characteristic predicting method as set forth in claim 1, which further comprises the steps of:

deriving said space occupied rate, said electrostatic factor and said steric factor for each of said component spaces forming said molecule surrounding space of each of a plurality of molecules, the reaction characteristics of which are to be predicted;

generating a plurality of sets of input data corresponding to said plurality of component spaces of each of said plurality of molecules, each set of said plurality of sets of input data being formed by said space occupied rate, said electrostatic factor and said steric factor; and

processing said plurality of sets of generated input data in accordance with a technique of a self-organizing neural network to display the processed result on a reaction characteristic predicting map indicative of reaction characteristics of said plurality of molecules.

15. A molecular reaction characteristic predicting method as set forth in claim 14, which further comprises the step of:

deriving said space occupied rate, said electrostatic factor and said steric factor for each of atoms of a plurality of molecules, the reaction characteristics of which are to be

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predicted;

generating a plurality of sets of input data corresponding to said atoms of each of said plurality of molecules, each set of said plurality of sets of input data being formed by said space occupied rate, said electrostatic factor and said steric factor; and

processing said plurality of sets of generated input data in accordance with a technique of a self-organizing neural network to display the processed result on a reaction characteristic predicting map indicative of reaction characteristics of said plurality of molecules.

16. A molecular reaction characteristic predicting method as set forth in claim 14, wherein said self-organizing neural network is a Kohonen neural network, and said reaction characteristic predicting map is a Kohonen map.

17. A molecular reaction characteristic predicting method as set forth in claim 16, wherein said Kohonen map is displayed so as to be plane.

18. A molecular reaction characteristic predicting method comprising the steps of:

describing atomic spherical surfaces, each of which surrounds a corresponding one of atoms of a molecule;

assuming that a portion of each of said atomic spherical surfaces intersecting the atomic spherical surfaces of other atoms of said molecule is an interior spherical surface;

assuming that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier spherical surface;

providing probe points on each of said atomic spherical surfaces at regular intervals;

deriving a rate of occupied space as a space occupied rate of a corresponding one of said atoms, for each of said atoms;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of said atoms of

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said molecule, for each of said probe points on said frontier spherical surface of each of said atoms;

deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said atoms, as an electrostatic factor of said corresponding one of said atoms;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said atoms;

deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said atoms, as a steric factor of said corresponding one of said atoms;

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said atoms; and

predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said atoms.

19. A reaction characteristic predicting map for predicting a reaction characteristic of a molecule, wherein referring to a molecular reaction characteristic predicting method for predicting a reaction characteristic of a molecule, said method comprising the steps of:

setting a molecule surrounding surface so as to be reflected in a spatial dimension of a molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces;

assuming that a portion of each of said component surrounding surfaces on said molecule surrounding surface

is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals; deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces, and predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said component spaces,

said space occupied rate, said electrostatic factor and said steric factor are derived for each of said component spaces forming said molecular surrounding space of each of a plurality of molecules, the reaction characteristics of which are to be predicted,

a plurality of sets of input data are generated so as to correspond to said plurality of component spaces of each of said

plurality of molecules, each set of said plurality of sets of input data being formed by said space occupied rate, said electrostatic factor and said steric factor,

said plurality of sets of generated input data are processed in accordance with a technique of a self-organizing neural network, and

the processed result is displayed so as to indicate reaction characteristics of said plurality of molecules.

20. A computer-readable storage medium having stored a program for predicting a reaction characteristic of a molecule, said program carrying out a process comprising the steps of:

setting a molecule surrounding surface so as to be reflected in a spatial dimension of a molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces;

assuming that a portion of each of said component surrounding surfaces on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces, and predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said component spaces.

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